Bogomol'nyi bound and screw dislocations in a mesoscopic smectic-A

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The de Gennes free energy functional of an infinite smectic-A liquid crystal at the dual point is shown to be topological and to depend only on the number of screw dislocations and the anisotropy. This result generalizes the existence of a Bogomol'nyi bound to an anisotropic system. The role of the boundary of a finite mesoscopic smectic is to provide a mechanism for the existence of thermodynamically stable screw dislocations. We obtain a closed expression for the corresponding free energy and a relation between the applied twist and the number of screw dislocations.

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A successful and striking analogy between different phases of a liquid crystal and those of a superconductor has been proposed by de Gennes back in 1972 [1]. It provides an example of how geometric and topological considerations lead to similar behaviours in two different physical systems [2]. This analogy has been further used by Renn and Lubensky to predict a new phase called the Twist Grain Boundary (TGB) phase [3], whose existence has been experimentally confirmed [4, 5, 6, 7, 8, 9, 10]. This phase is the liquid crystal analogue of the Abrikosov vortex lattice. It consists of screw dislocations that are topological defects. The TGB phase lies in between the smectic-A (SmA) and the cholesteric phase. In this letter, we show that the de Gennes free energy of a SmA has an integrability point at which it is topological. This leads to the existence of screw dislocation solutions, whose thermodynamic stability is obtained in the mesoscopic limit yet to be specified and for the geometry of an infinitely long cylinder of radius R. We characterize the smectic-A phase by the following set of length scales: the transverse and the longitudinal coherence lengths $\xi_\perp$ and $\xi_\parallel$, the twist penetration depth λ_T, and the wavenumber $q_s = \frac{2\pi}{d}$ of the density modulation of the nematogen molecules along the z-axis of the cylinder. The cholesteric pitch length defined by $L_p = \frac{2\pi}{k_0}$ [3] is generally larger than $\xi_\perp$. Here d is the separation between smectic layers and k_0 is the wavenumber of the Frank director in the cholesteric phase.

We first show that when written in a dimensionless form, the de Gennes free energy density $\mathcal{F}$ of an effective two-dimensional system is solely characterized by two dimensionless parameters, namely the twist Ginzburg parameter $\kappa = \frac{\lambda_T}{\xi_\perp}$ and the anisotropy parameter $\alpha = \sqrt{2}\kappa\xi_\parallel q_s \propto \xi_\parallel/\xi_\perp$. The dual point [11] is defined by $\kappa = 1/\sqrt{2}$. At this point and for a large system, the de Gennes free energy in the presence of a finite twist is a topological quantity that can be written

$$\int \mathcal{F} = 2\pi l(1-\alpha^2), \tag{1}$$

where the integer l accounts for the number of screw dislocations. This expression corresponds to the Bogomol'nyi bound [12] for the liquid crystal. However, from (1) it appears that there is no mechanism to select the number l of defects, and the free energy is minimum for $l = 0$. A way to thermodynamically stabilize solutions with $l \neq 0$ is to consider a mesoscopic finite size smectic, just like the unconventional vortex patterns obtained in mesoscopic superconductors [13]. A mesoscopic smectic-A for the geometry of a cylinder of radius R is characterized by $R \ll L_p$. Moreover, for $R > \xi_\perp$, we show that for a wide range of parameters k_0 and α, a mesoscopic SmA can accommodate screw dislocations and the selection mechanism for the equilibrium value of $l \neq 0$ is provided by the boundary conditions imposed on the total twist through the sample, in a way quite similar to the Little-Parks setup in superconducting rings.

We first consider some of the features of the SmA phase and the conditions of its description through the de Gennes free energy [1]. The order parameter that characterizes the SmA phase is the first harmonic of the density of the nematogen molecules. It can be written as $\Psi(\boldsymbol{r}) = |\Psi|e^{i\Phi}$ where $\Phi = q_s \boldsymbol{n}\cdot\boldsymbol{r}$. The unit vector $\boldsymbol{n}$ is the Frank director that specifies the molecular alignment. For a perfect SmA phase we have $\boldsymbol{n} = \{0,0,1\}$. The smectic planes are defined by $z = ld, (l \in \mathbb{Z})$, so that the phase $\Phi = 2\pi l$ [14, 15, 16]. A screw dislocation is a spiral staircase structure of the smectic planes [14, 15] characterized by a finite winding number. The free energy of a SmA is given by the sum of the Landau (F_L) and the Frank (F_F) contributions [16] which are, respectively:

$$F_L = \int r|\Psi|^2 + \frac{g}{2}|\Psi|^4 + C_\parallel|\frac{\partial\Psi}{\partial z}|^2 + C_\perp\left(|\frac{\partial\Psi}{\partial x}|^2 + |\frac{\partial\Psi}{\partial y}|^2\right) \tag{2}$$

$$F_F = \frac{1}{2}\int K_1(\boldsymbol{\nabla}\cdot\boldsymbol{n})^2 + K_2(\boldsymbol{n}.\boldsymbol{\nabla}\times\boldsymbol{n})^2 + K_3(\boldsymbol{n}\times\boldsymbol{\nabla}\times\boldsymbol{n})^2.$$

The Frank term F_F is the sum of energies associated to bend, twist and splay of $\boldsymbol{n}$. For a perfect SmA, the Frank energy vanishes. Hereafter we consider only the twist part in F_F. The de Gennes free energy [1, 16, 17] is obtained as the limit of the total free energy $F =$

$F_L + F_F$, when the Frank director $\boldsymbol{n}$ slightly deviates from the z-axis, namely $n_z \approx 1$ and both n_x and n_y are much smaller than n_z. This approximation together with the condition that $R \ll L_p$ defines the mesoscopic limit. The de Gennes free energy is thus given by [16]

$$\begin{aligned} F_{dG} &= \int r|\Psi|^2 + \frac{g}{2}|\Psi|^4 + C_{\|}|\frac{\partial \Psi}{\partial z}|^2 \\ &+ C_{\perp}|(\boldsymbol{\nabla}_{\perp} - iq_s\delta\boldsymbol{n}_{\perp})\Psi|^2 + \frac{K_2}{2}(\boldsymbol{\nabla}_{\perp}\times\delta\boldsymbol{n}_{\perp})^2, \end{aligned} \tag{3}$$

where $\boldsymbol{\nabla}_{\perp} = \{\partial_x, \partial_y\}$. We have introduced the two-dimensional vector $\delta\boldsymbol{n}_{\perp} = \boldsymbol{n} - \hat{\boldsymbol{z}}$. Since $\boldsymbol{n}^2 = 1$, at the lowest order $\delta\boldsymbol{n}_{\perp}$ lies in the x-y plane. The lengths $\xi_{\perp}$ and $\xi_{\|}$ over which the SmA order parameter changes respectively in the x-y plane and along the z-axis are obtained by comparing the corresponding gradient terms with the first term in the energy functional (3). This sets $\xi_{\perp} = \sqrt{C_{\perp}/|r|}$ and $\xi_{\|} = \sqrt{C_{\|}/|r|}$. The twist penetration depth is $\lambda_T = \sqrt{\frac{gK_2}{C_{\perp}q_s^2|r|}}$ [1, 3]. In the mean field approximation, only the coefficient r depends on temperature [1, 3, 17], so that the Ginzburg parameter $\kappa = \frac{\lambda_T}{\xi_{\perp}}$ is temperature independent. By rescaling all the lengths in units of $\sqrt{2}\lambda_T$, namely defining the scaling relations $\frac{r^2}{2g}\mathcal{F} = F_{dG}$, $\frac{-r}{g}|f|^2 = |\Psi|^2$, $\sqrt{2}\lambda_T\overline{x} = x$, $\sqrt{2}\lambda_T q_s = \overline{q}_s$ and $\overline{\boldsymbol{\nabla}}_{\perp} = \sqrt{2}\lambda_T\boldsymbol{\nabla}_{\perp}$, the de Gennes free energy (3) can be rewritten, up to a constant, in the dimensionless form

$$\begin{aligned} \mathcal{F} &= \kappa^2(|f|^2-1)^2 + \alpha^2|f|^2 + \\ &+ |(\overline{\boldsymbol{\nabla}}_{\perp} - i\overline{q}_s\delta\boldsymbol{n}_{\perp})f|^2 + \frac{1}{2}(\overline{\boldsymbol{\nabla}}_{\perp}\times\overline{q}_s\delta\boldsymbol{n}_{\perp})^2, \end{aligned} \tag{4}$$

where both f and $\delta\boldsymbol{n}_{\perp}$ do not depend on z. The anisotropy parameter $\alpha^2 = 2\kappa^2 q_s^2\xi_{\|}^2 = \overline{q}_s^2 C_{\|}/C_{\perp}$ contains $|r|$ and it is therefore temperature dependent. The expression (4) is analogous to the dimensionless Ginzburg-Landau free energy density of a two-dimensional superconductor in a magnetic field [18, 19], except for the additional term $\alpha^2|f|^2$. This term is proportional to $1/d^2$, and it accounts for the interaction between the nematogen density in SmA layers. The equilibrium equations are obtained by minimizing the functional (4) with respect to f^* and $\delta\boldsymbol{n}_{\perp}$. It gives

$$\begin{aligned} |\overline{\boldsymbol{\nabla}}_{\perp} - iq_s\delta\boldsymbol{n}_{\perp}|^2 f &= 2\kappa^2 f(1-|f|^2) - \alpha^2 f \\ \overline{\boldsymbol{\nabla}}_{\perp}\times(\overline{\boldsymbol{\nabla}}_{\perp}\times\overline{q}_s\delta\boldsymbol{n}_{\perp}) &= 2\boldsymbol{j}. \end{aligned} \tag{5}$$

The second relation is the liquid crystal analogue of the Maxwell-Ampère equation. It is written in terms of the two-dimensional liquid crystal current density, defined by $\boldsymbol{j} = Im(f^*\overline{\boldsymbol{\nabla}}_{\perp}f) - |f|^2\overline{q}_s\delta\boldsymbol{n}_{\perp}$. This current density vanishes for a perfect smectic. Using the phase of the SmA order parameter, it can also be written as $\boldsymbol{j} = |f|^2(\overline{\boldsymbol{\nabla}}_{\perp}\Phi - \overline{q}_s\delta\boldsymbol{n}_{\perp})$. In a superconductor, the vanishing of the in-plane circulation of the current density around a closed contour Γ implies the quantization of the magnetic flux. Similarly, in a SmA the vanishing of the circulation of the two-dimensional current density $\boldsymbol{j}$ around a closed contour implies that the smectic planes are lifted by an integer multiple of the layer separation d. We define the liquid crystal analogue of the London fluxoid by

$$\oint_{\Gamma}\overline{\boldsymbol{\nabla}}_{\perp}\Phi.d\overline{\boldsymbol{l}} = \oint_{\Gamma}(\frac{\boldsymbol{j}}{|f|^2} + \overline{q}_s\delta\boldsymbol{n}_{\perp}).d\overline{\boldsymbol{l}} = 2\pi l, \tag{6}$$

where l is an integer. We now make use of the following identity which holds in two dimensions only

$$|(\overline{\boldsymbol{\nabla}}_{\perp} - i\overline{q}_s\delta\boldsymbol{n}_{\perp})f|^2 = |\overline{\mathcal{D}}f|^2 + (\overline{\boldsymbol{\nabla}}_{\perp}\times\boldsymbol{j}) + |\overline{\boldsymbol{\nabla}}_{\perp}\times\overline{q}_s\delta\boldsymbol{n}_{\perp}||f|^2. \tag{7}$$

The scalar operator $\overline{\mathcal{D}}$ is defined by $\overline{\mathcal{D}} = \partial_{\overline{x}} + i\partial_{\overline{y}} - i\overline{q}_s(\delta n_x + i\delta n_y)$. We denote by Ω the cross-sectional area of the cylinder and by $\partial\Omega$ its boundary. We set boundary conditions by imposing that the system behaves as a perfect smectic at large distances, namely $|f| \to 1$ and $\boldsymbol{j} \to 0$ on $\partial\Omega$. Making use of those boundary conditions and of the identity (7), the free energy (4) at the dual point $\kappa = 1/\sqrt{2}$ can be written, up to a constant, as

$$\begin{aligned} \int_{\Omega}\mathcal{F} &= \int_{\Omega}\frac{1}{2}\left(1 - |f|^2 - \alpha^2 - |\overline{\boldsymbol{\nabla}}_{\perp}\times\overline{q}_s\delta\boldsymbol{n}_{\perp}|\right)^2 + |\overline{\mathcal{D}}f|^2 \\ &+ (1-\alpha^2)\oint_{\partial\Omega}(\frac{\boldsymbol{j}}{|f|^2} + \overline{q}_s\delta\boldsymbol{n}_{\perp}).d\overline{\boldsymbol{l}}. \end{aligned} \tag{8}$$

The boundary integral results from both the Stokes theorem and the boundary conditions. Making use of the relation (6), it is reduced to the constant term $2\pi l(1-\alpha^2)$. Then the free energy (8) is reduced to the sum of two positive terms. It is minimum when each of them vanishes, so that the minimum free energy is given by the so-called Bogomol'nyi bound (1) and the corresponding field configurations (5) are now solutions of the Bogomol'nyi like equations [12]

$$\overline{\mathcal{D}}f = 0, \text{ and } |\overline{\boldsymbol{\nabla}}_{\perp}\times\overline{q}_s\delta\boldsymbol{n}_{\perp}| + \alpha^2 = 1 - |f|^2. \tag{9}$$

It is important at this point to notice the role played by the nonlinear term in the free energy (4) in order to reach the Bogomol'nyi bound. The second equation in (9) expresses the dual relation between the twist and $|f|$. By eliminating the twist between these two equations, we obtain for $|f|$ the nonlinear equation $\overline{\nabla}_{\perp}^2 ln|f|^2 = 2(\alpha^2 + |f|^2 - 1)$. For $\alpha = 0$, it is a Liouville equation which is known [20] to admit families of vortex solutions characterized by the winding number l that appears in the free energy (1). The existence of a Bogomol'nyi bound for the de Gennes free energy of a SmA and the equations (9) are one of the main results of this letter.

For an infinite system there is no mechanism to select the number l of screw dislocations. The boundary of a finite mesoscopic SmA introduces such a mechanism that determines the value of l corresponding to stable screw

dislocation solutions as a function of the twist. In a finite system, the order parameter is not equal to 1 at the boundary, so that the boundary conditions used to derive (9) are not generally satisfied. Hence, the identification of the boundary integral in (8) with the fluxoid (6) is no longer possible and the free energy cannot be minimized just by using the Bogomol'nyi equations (9). To fix the boundary conditions for a finite system, we impose that the flux of the twist of the SmA through the cylinder is equal to the flux of a cholesteric in the same geometry. To implement it, we consider first the expression of the director $\boldsymbol{n}$ in the cholesteric phase [3, 16] given by $\boldsymbol{n}_{ch}(\boldsymbol{x}) = (0, sink_0x, cosk_0x)$ and obtained by minimizing the cholesteric free energy $F_{ch} = F_F - K_2 k_0 \int (\boldsymbol{n}\cdot\boldsymbol{\nabla}\times\boldsymbol{n})$. The flux of the twist through a cylinder of radius R is given by $\pi R^2 \boldsymbol{n}_{ch}\cdot\boldsymbol{\nabla}\times\boldsymbol{n}_{ch} = \pi R^2 k_0$. And because the total flux of the twist of the SmA is $2\pi R\delta n_\perp(R)$, we have

$$\delta\boldsymbol{n}_\perp(R) = \delta n_\perp(R)\hat{\boldsymbol{\theta}} = \frac{k_0 R}{2}\hat{\boldsymbol{\theta}} = \frac{\pi R}{L_p}\hat{\boldsymbol{\theta}}. \qquad (10)$$

This boundary condition disregards edge dislocations [21, 22]. For the geometry of a cylinder, the current density $\boldsymbol{j}$ has only an azimuthal component. We note that on the boundary, $\overline{\boldsymbol{\nabla}}_\perp\Phi|_{\partial\Omega} = l/\overline{R}$, so that for

$$l \leq \frac{q_s k_0 R^2}{2} = \Phi_{ch} \qquad (11)$$

the current density $j_\theta(R)$ is negative. Moreover, since the current density is positive at the core of a screw dislocation, there exists a circle along which the current density vanishes. It allows to split the domain Ω into two concentric subdomains $\Omega = \Omega_1 \cup \Omega_2$, so that the boundary $\partial\Omega_1$ is the zero current density line. The system can now be divided into a bulk (Ω_1) and an edge region (Ω_2). We neglect the interaction between the screw dislocation and the edge current, so that the total free energy density of the system is now given by $\mathcal{F} = \mathcal{F}(\Omega_1) + \mathcal{F}(\Omega_2)$. Since the boundary $\partial\Omega_1$ is the zero current line, we can approximate $\mathcal{F}(\Omega_1)$ by the Bogomol'nyi bound (1) [19]. For the edge free energy, we use expression (4) integrated over Ω_2. The twist $\mathcal{T}(\overline{r}) = \overline{\boldsymbol{\nabla}}_\perp \times \overline{q}_s\delta\boldsymbol{n}_\perp$ enters the system up to a distance of order 1 in units of $\lambda_T\sqrt{2}$ [1]. Therefore, it decreases from the boundary at $r = R$ with a behaviour well described by

$$\mathcal{T}(\overline{r}) = \overline{\boldsymbol{\nabla}}_\perp \times \overline{q}_s\delta\boldsymbol{n}_\perp = \frac{\Phi_{ch} - l}{\overline{R}} e^{-(\overline{R}-\overline{r})}, \qquad (12)$$

where Φ_{ch} is defined by (11). The value at the boundary $\mathcal{T}(\overline{R}) = (\Phi_{ch} - l)/\overline{R}$ results from the expression of the total twist $2\pi\Phi_{ch}$ as a sum $2\pi l + \int_{\Omega_2}\mathcal{T}(\overline{r})$ of the twists associated respectively to the dislocations in the subdomain Ω_1 and to the contribution of the subdomain Ω_2. The twist contribution to the free energy in expression (4) is thus given by $\int_{\Omega_2}\frac{1}{2}(\overline{\boldsymbol{\nabla}}_\perp\times\overline{q}_s\delta\boldsymbol{n}_\perp)^2 = (l-\Phi_{ch})^2/4\overline{R}$. Along the same line of arguments, the quantity $\boldsymbol{j}/|f|^2 = \overline{\boldsymbol{\nabla}}_\perp\Phi - \overline{q}_s\delta\boldsymbol{n}_\perp$ is such that $\int_{\Omega_2}\left((\overline{\boldsymbol{\nabla}}_\perp\times\boldsymbol{j})/|f|^2 + \mathcal{T}(\overline{r})\right) = 0$. Then, $-\boldsymbol{j}/|f|^2$ restricted to the subdomain Ω_2 is also given by (12). At the dual point we have $\lambda_T = \xi_\perp/\sqrt{2}$, so that the amplitude of the nematogen density modulation f saturates to its equilibrium value (undistorted SmA) over a distance $\lambda_T\sqrt{2}$. With the help of these observations, we estimate $\mathcal{F}(\Omega_2)$ using a variational ansatz, namely that the modulus $|f|$ has a constant value f_0 over a ring of width $\lambda_T\sqrt{2}$, included in Ω_2, so that the term $\overline{\boldsymbol{\nabla}}_\perp|f||_{\partial\Omega} = 0$ [19]. This leads to an edge energy of the form:

$$\begin{aligned}\int_{\Omega_2}\mathcal{F} &= \frac{(l-\Phi_{ch})^2}{4\overline{R}} + \qquad (13)\\ &+ \pi\overline{R}\left(\frac{(l-\Phi_{ch})^2}{\overline{R}^2}f_0^2 + (1-f_0^2)^2 + 2\alpha^2 f_0^2\right).\end{aligned}$$

We then minimize with respect to f_0, which yields $2(1-f_0^2) = \frac{(l-\Phi_{ch})^2}{\overline{R}^2} + 2\alpha^2$. The corresponding expression for the extremum value of the edge free energy (14) together with the bulk term (1) gives for the total free energy

$$\begin{aligned}F_l(\Phi_{ch}) &= 2\pi l(1-\alpha^2) + \frac{\pi}{\overline{R}}[\frac{3}{2}(l-\Phi_{ch})^2 + 2\overline{R}^2\alpha^2]\\ &- \frac{\pi}{4\overline{R}^3}[(l-\Phi_{ch})^2 + 2\overline{R}^2\alpha^2]^2. \qquad (14)\end{aligned}$$

This relation constitutes the second main result of this letter. In the limit of a radius $R \gg \lambda_T$, the quartic term becomes negligible compared to the quadratic one, so that the Φ_{ch}-dependence of the total free energy appears as the envelop of a family of parabolae each indexed by the integer l. The system chooses its winding number l in order to minimize the free energy. This provides a relation between the number l of screw dislocations and the twist Φ_{ch} given by the integer part $l = [\Phi_{ch} - \frac{2}{3}\overline{R}(1-\alpha^2)]$. The entrance of the $(l+1)$-th screw dislocation occurs for a value of the twist, so that $F_l = F_{l+1}$. The entrance of the first dislocation is thus given by $\Phi_{ch} = \frac{1}{2} + \frac{2}{3}\overline{R}(1-\alpha^2)$, which according to (11) gives for the corresponding twist the expression $k_0 = \frac{1}{q_s R}\left(\frac{1}{R} + \frac{4(1-\alpha^2)}{3\sqrt{2}\lambda_T}\right)$. The highest value $k_0^{(c)}$ of the twist that allows the entrance of screw dislocations corresponds to the critical value at which the system becomes cholesteric. It is given by $k_0^{(c)} = \sqrt{\frac{r^2}{gK_2}}$ [3] and it corresponds to $\Phi_{ch}^{(c)} = \overline{R}^2/\sqrt{2}$. Using this expression in (11), we obtain a bound for the largest number of screw dislocations that a mesoscopic sample can accomodate. All these results are summarized in Figure 1, which presents the behaviour of the free energy F_l as a function of Φ_{ch}. In deriving the expression (14), we have implicitely assumed that the parameters $\Phi_{ch} \propto k_0$ and α^2 can be changed independently. Nevertheless, it has been shown experimentally [5] that both k_0 and α^2 depend on temperature. However, it has been argued that

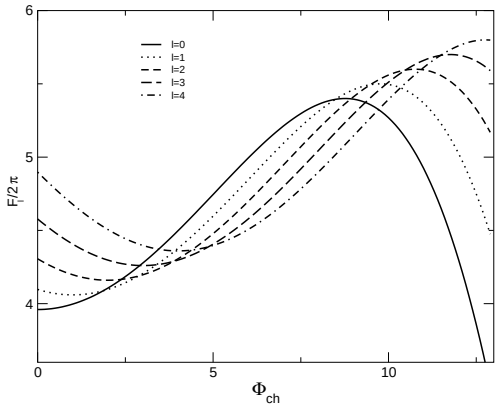

FIG. 1: *Free energy F_l of a mesoscopic SmA as a function of the twist Φ_{ch} as given by (14) with $\overline{R} = 8$ and $\alpha^2 = 0.9$.*

k_0 might also be changed at fixed temperature [3, 23]. Since we do not know the exact temperature dependence of k_0 and α^2, we have presented in Figure 2 the phase diagram of a mesoscopic SmA in the Φ_{ch}-α^2 plane. It exhibits finite areas where screw dislocations are energetically stable. In conclusion, we have shown that the

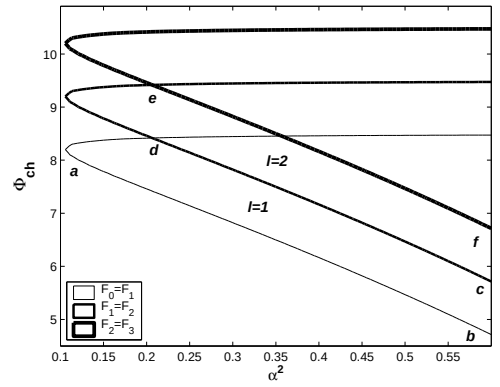

FIG. 2: *Phase diagram in the Φ_{ch}-α^2 plane, of a mesoscopic smectic-A with screw dislocations ($l = 1, 2, 3$) and $\overline{R} = 8$. The region enclosed by a given contour corresponds to $F_{l+1} < F_l$ and a screw dislocation with winding number $l + 1$ is energetically favoured as compared to one with winding number l. Thus, in the area $(abcd)$, we have a $l = 1$ dislocation while the area $(dcfe)$ corresponds to $l = 2$. The critical twist $\Phi_{ch}^{(c)} = \overline{R}^2/\sqrt{2}$ (see text) at which the system becomes cholesteric is $\Phi_{ch}^{(c)} = 45.26$.*

de Gennes free energy of a smectic-A is characterized by two dimensionless parameters κ and the anisotropy α. At the dual point $\kappa = 1/\sqrt{2}$, the free energy is topological and it saturates the Bogomol'nyi bound. The role of the boundary of a finite size mesoscopic smectic is to provide a mechanism for the existence of stable screw dislocations. The Bogomol'nyi equations (9) have been obtained without any specific assumption on the nature of the twist field. Therefore, they share some similarities with those obtained in other situations like mesoscopic superconductors [19], Chern-Simons [24] and Yang-Mills [25] field theories. These analogies can be pushed further towards other anisotropic layered systems like anisotropic High-T_c superconductors or double layer quantum Hall systems [26].

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